REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	03/31/05	Final 07/01/01-03/31/05

4. TITLE AND SUBTITLE

Final Progress Report of Spin Coherence and Magnetization Transport in Nanometer-Scale Structures, DARPA/ARO Research Agreement No. DAAD19-01-C-0060

5. FUNDING NUMBERS

DAAD19-01-C-0060

6. AUTHOR(S)

Barbara Jones, Donald Eigler, Andreas Heinrich, and Antonio Castro Neto. Edited and compiled by Barbara Jones.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

IBM Almaden Research Center
650 Harry Road
San Jose, CA 95120-6099

8. PERFORMING ORGANIZATION REPORT NUMBER

3156-04

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

42673.1-PH-QC

11. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12a. DISTRIBUTION AVAILABILITY STATEMENT

Approved for public release; distribution unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Enclosed is the final report of Research Agreement No. DAAD19-01-C-0060. Highlights of the full reporting period include the construction of a custom-built low-temperature high magnetic field STM with ultra high vacuum sample preparation, the first of its kind. Key experimental results were obtained in STM studies of Kondo lattice and in behavior of Kondo effect in magnetic fields. IBM achieved its milestone of demonstrating single-atom spin-flip spectroscopy, published in Science (2004). IBM finalized its work on the spectroscopic properties of physisorbed molecular hydrogen in nanoscopic junctions, finding unusual excitations. Finally, IBM found when Mn atoms were placed near the edge of thin oxide islands, an enhanced zero bias conductance emerged, a notably clear manifestation of the Kondo effect. Theoretically, the IBM-Boston University collaboration completed the formulation of a comprehensive theory of STM/magnetic atom/surface states/bulk interactions, and found very good agreement with experiment. A surprising result is that the surface Kondo effect is primarily an effect of bulk electrons. Detailed comparisons show that the description of STM data can only be done with the use of sophisticated ab initio band structure calculations. IBM also has theoretical results for Magnetic Tunnel Junctions for spin-sensitive STM tips, including effects of current-induced spin torques.

14. SUBJECT TERMS

Kondo, Anderson model, STM, magnetic fields, Kondo lattice, atomic manipulation, Fano resonance, spin-flip spectroscopy

15. NUMBER OF PAGES

29

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

Final Progress Report

**Spin Coherence and Magnetization Transport
in Nanometer-Scale Structures**

**DARPA/ARO Research Agreement
No. DAAD19-01-C-0060**

**IBM
and subcontractor Boston University**

List of Illustrations with page numbers

Table of Contents

I. Statement of Problem Studied

IBM, working together with Boston University (BU), set out a concerted research program with the goal of laying the foundations for novel devices and computing technologies, both quantum and classical, which are based on the manipulation of spins and magnetization transport in nanometer-scale structures. The work involved preparing the systems of magnetic impurities, controlling and detecting the atoms and spins, and understanding the results via the overlapping theory work. Leveraging IBM's experimental facilities and using IBM and BU's established expertise in STM nanoassembly and theoretical modeling of spin dynamics targeted two main goals:

- Establish a fundamental understanding of the spin dynamics of nanoassembled structures
- Explore the potential for coupled-spin nanostructures that transport and process information

As an overall challenge, it is not at all clear that running an electrical current through a nanometer scale structure is the optimum way to transport information in such dimensions. Power dissipation, localization, and electromigration are all problems that have to be reexamined in such small structures. An alternative method for transporting information and doing logical operations on that information is to use the electron's spin degree of freedom as opposed to its momentum degrees of freedom. IBM and BU wanted to understand the physics of transporting and doing logic on information using just the spin degree of freedom. To achieve this broad long-term goal, IBM built a new low-temperature (0.6 K) high-field (7.5T) STM for studying the spin physics of small structures while simultaneously conducting studies with its existing low-temperature STM.

IBM's experimental technical goals included:

- Demonstrate spin polarization of tunneling current when tunneling into the bound-state excitation at a magnetic impurity atom on the surface of a superconductor, metal, or insulator

- Measurement of the g value of a single atom

- Measure spectrum of spin excitations in nanoassembled magnetic structures.

- Build a foundation of knowledge concerning the magnetic properties of nanostructures

- Explore device structures for information transport and processing which utilize the spin degree of freedom of the structures

- Explore the use of tips with specialized materials for both tip and terminating atomic-scale structures as a sensitive probe of the local spin polarization of nanometer scale systems

On the theory side, the ambitious goals were to combine three complex systems in order to understand and predict STM measurements: 1) the STM tip, and its interactions with the surface atoms and adatoms; 2) adatoms, with typically many-body behavior of Kondo effects, magnetism, or both; and 3) the host with bulk states and surface states. Each of these three is a project in of itself, and then to combine them into one Hamiltonian and obtain solutions was the grand challenge of IBM and BU working together. In the process of this, BU also had to develop a local density functional approach to the surface states, and especially wave functions as they tail into the vacuum as much as 16 or more Angstroms away. So IBM and BU's calculations were both many-body analytic, and also heavily numerical.

IBM also was interested in developing structures for STM tips for spin detection. IBM's theory approach structure of choice was a nanoscale (in all dimensions) magnetic tunnel junction, and a portion of the theory work was to develop a working model for magnetic tunnel junctions in which interface effects were predominant, and see the effects on spin tunneling current.

The third aspect of the theory at IBM was to explore any effects of current-induced magnetization reversal, since a magnetic tunnel junction with nanoscale dimensions in all three directions on an STM tip is nothing more than a magnetic sandwich in a nanowire. Such a structure on an STM tip would easily experience currents in the range of current-induced magnetization reversal, and IBM wished to explore how to predict and control these effects.

IBM and BU's longer-range technical goals for spin-current devices were:

- Develop predictive many-body theory for the transition from isolated-impurity to spin-coupled states of impurities in nanoscale structures.

- Determine controlling factors for propagation of spin coherence information between Kondo impurities in atomic nanostructures.

II. Summary of Results

A. Experiment

Summary

This reporting period saw progress in three aspects of IBM's experimental program to probe and manipulate the magnetic properties of nano-scale structures with the scanning tunneling microscope (STM).

Single-atom spin-flip spectroscopy

First, IBM was able to achieve the milestone of single-atom spin-flip spectroscopy with the STM. IBM demonstrated the ability to measure the energy required to flip the spin of single adsorbed atoms. A low-temperature, high-magnetic-field scanning tunneling microscope was used to measure the spin excitation spectra of individual Mn atoms adsorbed on Al2O3 islands on a NiAl surface. IBM found pronounced variations of the spin-flip spectra for Mn atoms in different local environments. In particular, Mn atoms were placed on thin oxide films and g values in the range of 1.80 to 2.00 were measured. This is the first step to fulfilling the goal of directly measuring the magnetic excitations of magnetic nanostructures in a solid state environment. This work was made possible because of the successful construction and use of the world's first low-temperature (T<1K) high-magnetic-field STM with ultra-high vacuum sample preparation.

Second, IBM studied the influence of the solid state environment on the magnetic excitation spectra of single Mn atoms. When Mn atoms were placed near the edge of thin oxide islands IBMfound the emergence of an enhanced zero bias conductance. This manifestation of the Kondo effect is similar to the Kondo effect in other nanostructures and notably clearer than previous STM investigations.

A paper encompassing both aspects of the magnetic excitations of individual atoms has been published by *Science* Magazine in November of 2004.

Third, IBM finalized its work on the spectroscopic properties of physisorbed molecular hydrogen in nanoscopic junctions. While IBM's results were obtained in an STM these findings are equally important for the emerging field of molecular electronics. A manuscript has been submitted to *Phyical Review Letters* and is currently under review.

Details

In this reporting period IBM reached the milestone of using a scanning tunneling microscope (STM) to measure the Zeeman energy of individual Mn atoms in a solid-state environment. These measurements utilized inelastic tunneling spectroscopy (IETS), a technique originally developed to measure vibrational excitations of single molecules. This constitutes significant progress towards the use of STM for the measurement of the magnetic properties of artificial and self-assembled nanostructures.

The energy scale associated with magnetic excitations of atoms is the Zeeman energy, $\Delta = g\mu_B H$. For a free electron with a g value of 2.0 and for magnetic fields achievable in a lab of order 10T this energy is of order 1 meV. To resolve such a small energy scale in a tunnel junction it is necessary to work at temperatures below 1K. In the last reporting period IBM described the successful design, construction, and operation of the world's first STM with such temperature and magnetic field requirements and ultra-high vacuum sample preparation. This novel STM was used extensively in this period and is operating at and above expectations.

IBM found previously that a magnetic atom directly on top of a metal substrate interacts too strongly with the conduction electrons in the substrate to show IETS spin-flip spectra. IBM therefore chose a sample configuration consisting of insulating Al_2O_3 on a NiAl (110) metallic substrate. This oxide is thin enough to allow stable tunneling even at low bias voltages, but thick enough to place the adsorbate away from the substrate electrons to avoid screening of the adsorbate's magnetic moment, and consequently to allow spin-flip spectroscopy. The NiAl sample is prepared so that it is partly covered with well-ordered 0.5 nm thick oxide, and the rest of the surface exposes atomically clean NiAl (110) metal. One of the key features of the new STM is the fact that IBM can transfer samples directly from a room-temperature vacuum chamber, where the samples are prepared, into the cold STM. This assures atomic cleanliness of the sample in the STM.

When the tip was positioned over a Mn atom on oxide IBM found a marked magnetic-field dependence of the conductance. At IBM's maximum field of $B = 7\,T$ the conductance was reduced near zero bias, with symmetric steps up to a 20% higher conductance at the Zeeman energy of $|\Delta| = g\mu_B B \sim 0.8$ meV. These conductance steps were absent at $B = 0$. Furthermore, no conductance steps were observed when the tip was positioned over the bare oxide surface, over the bare metal surface, or over a Mn atom on the metal surface. The spatial extent of the conductance step (the IETS spin-flip signal) was found to be 1 nm in diameter, comparable to the atom's apparent lateral extent in the corresponding STM topograph.

The measured Zeeman splitting was found to be proportional to the magnetic field and well described with $g = 1.88 \pm 0.02$. Other Mn atoms closer to the edge of oxide patches showed significantly different g value in the range of $g = 1.80$ to 2.00. The only difference between these Mn atoms is the local environment: they have different lateral distances to bare metal region, they may sit at different binding sites in the oxide unit cell, and perhaps more importantly, IBM expect the oxide patch to show reconstruction near the boundary to minimize its energy. It is one of the great strengths of the STM to be able to distinguish differences in these IETS spectra on neighboring atoms.

A second experimental advance in this reporting period was the study of magnetic moments interacting strongly with their environment, an important step towards the goal of coupling magnetic moments to each other. Many magnetic atoms deposited directly onto a metal substrate were shown in previous STM studies to lead to Kondo resonances. However, rather than simply resulting in the expected enhanced zero-bias conductance,

the Kondo effect was generally obscured by the interference of many tunneling paths resulting in more complicated Fano lineshapes.

IBM found that Mn atoms on oxide that are laterally near metal-oxide interfaces can exhibit spectra that differ markedly from the spin-flip IETS of isolated Mn atoms on oxide. These spectra show the hallmarks of Kondo resonances: a narrow conductance peak with Lorentzian shape at zero bias. IBM found Kondo temperatures between $T_K \sim 3$ K and $T_K \sim 6$ K for Mn atoms in different local environments. These Kondo temperatures are one order of magnitude smaller than previous Kondo systems investigated by STM. IBM believes these lower Kondo temperatures are a manifestation of the reduced coupling of the magnetic moments to the conduction electrons due to the thin oxide film. For the first time in STM studies of Kondo systems, IBM was able to measure the splitting of the Kondo resonance in magnetic fields.

IBM also attempted to perform controlled manipulation of Mn atoms on the oxide film with the STM as part of IBM's effort towards its next milestone of using the STM to probe the magnetic properties of artificially assembled nanomagnets. These manipulations turned out to be significantly more difficult than moving atoms on noble metal surfaces for two reasons. First, IBM has to keep the tip far away from the Mn on oxide because there is a high probability of transferring the Mn atom to the tip in an uncontrolled fashion. It is therefore not possible to slide Mn on oxide with atomic-scale control. Second, the Al_2O_3 on NiAl (110) has a rather complicated structure; it is not commensurate with the metal substrate and exposes different binding sites for adsorbates in a large surface unit-cell.

IBM has succeeded in moving Mn atoms between locations on the surface by first transferring them to the STM tip and then transferring them back to the surface at the desired final location by using an appropriate voltage pulse. This is notable in part because it is the first time that metal atoms have been reversibly transferred between a surface and the STM tip. Unfortunately this process has worked reliably with only a select few STM tips, and IBM is working to understand if this process can be made more reliable. During these studies of manipulation of Mn on the thin insulator IBM discovered a major drawback for using Al_2O_3 on NiAl (110) as the substrate for the atomically controlled assembly of nanomagnetic structures: when IBM dropped off a Mn atom from the tip in the vicinity of a pre-existing Mn atom the original atom would always disappear. Of course that makes the controlled assembly of dimers and larger nanostructures impossible at the present. IBM believes that other thin insulating substrates might be better suited for the manipulation of spins and is looking into promising alternatives to Al_2O_3 on NiAl (110).

A third experimental avenue in this reporting period was IBM's work on physisorbed Hydrogen in the junction of a low temperature STM. IBM found previously that H_2 accumulates in the tip sample junction of the cold (10K and below) STM and gives rise to interesting spectra. In this period IBM was able to conclusively attribute the BCS gap-like and the negative differential resistance spectra to the same physical origin: inelastic excitations with saturation of a two-state system. In brief, IBM observed a two-state switching of the elastic conductivity of the tunnel junction when it is excited by an inelastic scattering event with the tunneling electron. This is always the case in inelastic tunneling spectroscopy; however in all previous studies the lifetime of that excited state

was so short that subsequent tunneling electrons would always see the ground state. Any time that lifetimes of excited states occur in the range of the average time between tunneling events, similar spectroscopic signatures to the ones IBM measures must be expected. IBM therefore believes that this work is relevant to many fields of inelastic spectroscopies such as vibrational spectroscopy, and may be particularly important in explaining the observed changes in conductivity and negative differential resistance in candidate molecular electronics systems.

B. Theory results

1. BU Collaboration: A Comprehensive Theory of STM measurements of magnetic atoms on surfaces

Scanning tunneling microscopy (STM) has become one of the most basic tools for the manipulation of matter at the atomic scale. Although this experimental technique has reached a great level of maturity, the detailed theoretical understanding of experimental data is still incomplete and/or contradictory.

The most famous example of atomic manipulation is probably associated with the surface Kondo effect observed when transition metal ions (such as Co) are placed on a metallic surface (such as Cu(111)) [1]. The surface Kondo effect is the basis for the observation of surprising phenomena such as quantum corrals [2], and quantum mirages [3], and has attracted a lot of attention and interest in the last few years. The current understanding of these observations is based on the assumption that only surface states of Cu(111) are involved in the scattering of electron waves by the Co adatoms [4]. Nevertheless, various different experiments with Co atoms on Cu(100) surface (that does not have any surface state) [5], or with Co adatoms in Cu(111) put close to atomic surface steps (that affect the surface states) [6] have indicated that bulk (not surface) states are behind the surface Kondo effect. Meanwhile, the growing theoretical literature in the subject is heavily concentrated on the surface states alone.

The theoretical understanding of these effects is the main target of this collaboration between IBM-Almaden and Boston University (BU) researchers. The IBM-BU collaboration is characterized by the tight link between the experiments conducted at IBM-Almaden by Eigler's group and the theoretical group headed by Castro Neto (BU) and B. Jones (IBM). Furthermore, this research has a strong education content since the bulk of the work was developed by C.Y. Lin, a PhD student at BU, and is the basis of his PhD thesis.

In a STM experiment one measures the voltage V dependence of the tunneling current, I, that is, the so-called tunneling conductance, dI/dV , as a function of the lateral distance R between the tip and the Co adatom (the tip is kept at a distance Z from the surface), and the voltage V . At low temperatures, below a certain temperature TK called the Kondo temperature, the experimental data is fitted by [7]:

$$\frac{dI}{dV} - \left(\frac{dI}{dV}\right)_0 = A(R) \left\{ \frac{q^2(R) - 1 + 2q(R)\xi(V)}{\xi^2(V) + 1} \right\}, \qquad (1.1)$$

where the differential conductance with a subscript "0" refers to the background signal (proportional to the local density of states of the substrate), A(R) is the amplitude of the STM signal, q(R) is the Fano line shape parameter, and $\xi(V)$ is the dimensionless bias voltage that can be written as:

$$\xi(V) = \frac{eV + \bar{\epsilon}_a}{k_B T_K}, \qquad (1.2)$$

where $\bar{\epsilon}_a$ is a bias offset. Depending on the value of q the tunneling conductance changes shape as a function of V. This is called the Fano lineshape [8].

It is important to understand the basic physics involved in the problem: when a Co atom is placed on a Cu(111) surface it can, in principle, hybridize with the surface and bulk states of Cu. Since the hybridization occurs through well localized d-states of Co, the Coulomb energy is large leading to a strong magnetic scattering: the Kondo effect. The theory of the tunneling conductance [7] relates the basic measured experimental quantities (q, $\bar{\epsilon}_a$, TK) to microscopic quantities such as the hybridization energies between adatom d-state and the substrate, Vka, the STM tip and the substrate, tpk, and the hybridization energy between the STM tip and adatom, tpa. These hybridization energies are written in term of matrix elements between different wavefunctions. For instance,

$$V_{ka} = \int d^3r\ \psi_{\mathbf{k}}^*(\mathbf{r}) \left(H_0 + V_a(\mathbf{r})\right) \psi_a(\mathbf{r}), \qquad (1.3)$$

where k(r) is the substrate wavefunction scattered by the adatom potential, H0 refers to the bare metal surface, Va(r) is the adatom scattering potential, and $\psi_a(\mathbf{r})$ the adatom 3d orbital. Similar expressions are written for the tip hybridization energies, tpk and tpa, where the matrix elements are calculated between the tip and the substrate (adatom) wavefunction [9].

Since the STM tip can be controlled externally, one works in the linear response regime where the tip is weakly coupled to both the adatom and substrate. In this case, the physics of the problem is dominated by the hybridization of the adatom with the substrate and the STM is just a probe.

The starting point of the theoretical description of this problem is the Anderson impurity model [10]:

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} (V_{ka} c_{k\sigma}^\dagger c_a + V_{ka}^* c_a^\dagger c_{k\sigma}) + \sum_\sigma \epsilon_a c_{a\sigma}^\dagger c_{a\sigma} + U n_\uparrow n_\downarrow \quad (1.4)$$

where ϵ_k is the energy of the substrate electrons, $c_{k\sigma}^\dagger$ $(c_{k\sigma})$ creation (annihilation) for substrate electrons with momentum k and spin σ, ϵ_a is the energy of the d-orbital

adatom electrons, $c_{k\sigma}^{\dagger}$ $(c_{k\sigma})$ is the creation (annihilation) of adatom electrons with spin σ, and U is the Coulomb energy for double occupancy of the d-orbital $\left(n_{\sigma} = c_{a,\sigma}^{\dagger} c_{a,\sigma}\right)$.

In the limit when Vka is small when compared to the other energy scales in the problem (the Fermi energy, EF , and U) one can map (1.4), via a Schrieffer-Wolff transformation [11], onto the Kondo Hamiltonian that describes the problem of electronic spins being scattered by a localized magnetic moment. As BU showed, however, this is not the case in the problem of adatoms in metallic surfaces where the hybridization can be comparable to the other energy scales in the problem. So, strictly speaking, one is not dealing with a Kondo problem since charge fluctuations are important and hence one has to use the Anderson impurity Hamiltonian (1.4) instead of the Kondo Hamiltonian. Nevertheless, BU will follow the tradition and still call the effect as the surface Kondo effect.

One of the characteristics of the Anderson impurity model is the distinction between substrate and adatom wavefunctions. Although most theoretical works do not question the distinction made a priori between these quantum states, it turns out that this distinction is not completely natural. The reason is very simple: when an impurity atom is introduced in a metal, it hybridizes with the metallic states losing its identity. However, it leaves behind a phase shift δ_{k}/N in the original metallic states (N is the total number of atoms in the system). Thus, the impurity state cannot be really distinguished from the host states from the quantum mechanical point of view. Nevertheless, Anderson [10] makes the point that because the d-orbitals are a inner shell, the Coulomb energy U for double occupancy of those orbitals is large and they must be distinguished from metallic states where the Coulomb energy is strongly suppressed by screening effects. Thus, the distinction between these two types of states can only be clearly made when these states are orthogonal to each other so that the impurity does not cause a direct perturbation in the substrate spectrum. Nevertheless, even in metals where the electronic bands are generated out of d-orbitals (such as in the case of Cu), the strong metallic bonding leads to a large s-wave character of the bands and to very small overlap with the adatom d-orbitals (that is, these states are "naturally" orthogonal) [12]. Nevertheless, this orthogonality can only be distinguished a posteriori. In fact, BU has found, by direct numerical computation, that this is the case in the surface Kondo effect.

Finally, as pointed out by Anderson [10], the orthogonality of these states is not fundamental for the magnetic phenomenon which is essentially a local effect and all the subtleties associated with orthogonality become encapsulated into the hybridization matrix elements Vka which become phenomenological parameters to be obtained indirectly from the experiment. However, in trying to understand the STM experiments, and especially the role played by the surface and bulk states, BU cannot simply take these matrix elements as phenomenological parameters since BU would not be able to separate the contributions coming from the bulk and the surface of the Cu substrate. Thus, BU has performed microscopic calculations of these matrix elements starting from the electronic wavefunctions.

The theory of the STM response can be obtained by working at very low temperatures (below the Kondo temperature TK) and assuming a Fermi liquid picture of Nozieres [13] where the adatom is magnetically screened by the substrate electrons. In this case it can be shown that the Fano parameter in (1.1) is given by [7]:

$$q = \frac{t_{pa} + \operatorname{Re} F(E_F)}{\operatorname{Im} F(E_F)}, \tag{1.5}$$

where

$$F(\omega) = \sum_{\mathbf{k}} \frac{t_{pk} V_{ka}}{\omega - \epsilon_{\mathbf{k}} + i\eta}, \tag{1.6}$$

is the Green's function that describes the quantum mechanical interference between the different tunneling paths from the tip and the substrate to the adatom. The amplitude A(R) can be written as:

$$A(R) \propto |\operatorname{Im} F(E_F)|^2 . \tag{1.7}$$

Moreover, using field theoretical methods (the slave-boson technique [14]) IBM/BU calculate the Kondo temperature of the adatom directly from the Anderson impurity model (1.4) as

$$T_K = D \exp\{-\pi \epsilon_a / (2\Delta)\}, \tag{1.8}$$

where Δ is the d-level broadening and related to the hybridization energies by

$$\Delta = \pi \sum_{\mathbf{k}} |V_{ka}|^2 \delta(\epsilon_{\mathbf{k}} - E_F), \tag{1.9}$$

and D is the electron bandwidth. Notice, therefore, that the STM response depends mostly on the substrate-adatom hybridization energy Vka, which in its turn, depends on how the d-orbital of the adatom hybridizes with the surface and bulk states of the substrate.

IBM/BU's objective is to develop a consistent theory of these hybridization energies Vka that can explain the STM data. In order to accomplish this task, one has to calculate the wavefunction and spectrum for the bulk and surface states of the substrate and the adatom and their overlap as given in (1.3). From that, one further can calculate the STM response expressed in (1.1) through (1.5) and (1.7). This study will allow IBM/BU to investigate how bulk and/or surface states contribute to the surface Kondo effect. The understanding of this basic phenomenon will open doors for the description of basic physics at the atomic level that can be studied with STM techniques.

Results, initial model

In IBM/BU's first manuscript [15], BU considered the microscopic calculation of the hybridization matrix elements between the different wavefunctions in the problem (bulk, surface, impurity, and STM tip) with the smallest number of adjustable parameters. While the spectra for bulk and surface states is readily available in the literature [16], very little has been published on the actual form of the wavefunctions. Instead of embarking on a complicated calculation of wavefunctions via heavy numerical techniques, BU opted for a simpler approach that can provide quantitative results that can

be directly compared to the experiment as well as intuitive understanding of the problem. As IBM/BU showed, however, their simplified models have limitations in explaining the available STM data and more detailed work was required (see next section).

Metallic Cu is a very good metal with a nearly spherical Fermi surface except for the gaps in the (111) direction. These gaps have their origin in the periodic potential generated by the ions. Although the Cu states can be obtained from first principle calculations [16] IBM/BU adopted the nearly free electron approximation and model the bulk potential with a simple periodic function. Furthermore, in order to study the surface states IBM/BU consider a semi-infinite crystal where the bulk is located at $z < 0$ and the potential outside the crystal is given by the image potential [17]. In Fig. 2.1 is plotted the physical situation in the problem. The eigenfunctions and eigenenergies for the Schroedinger equation associated with this potential can be calculated exactly [17].
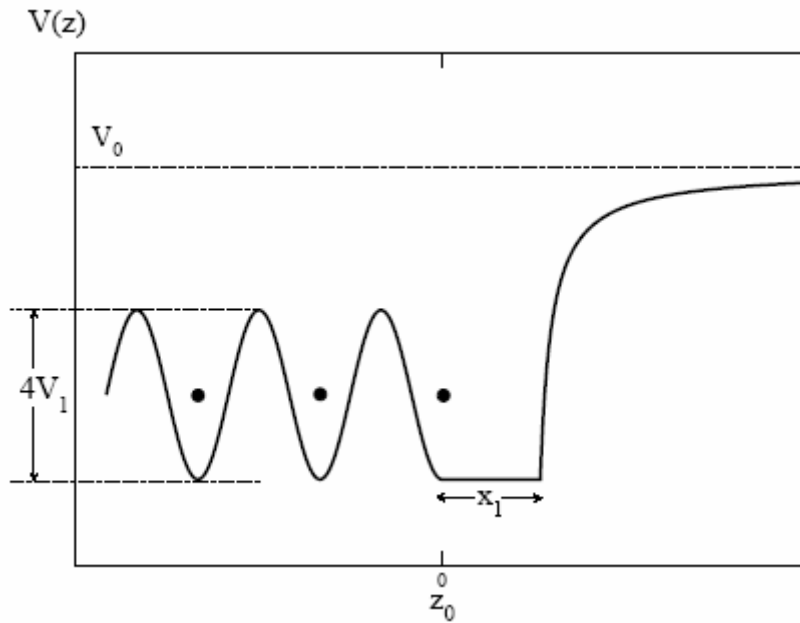

Figure 2.1: Plot of the image potential energy near a crystal surface. The solid dots are crystal atoms.

With just a few adjustable parameters like the strength of the periodic potential (V0 and V1 in Fig.2.1) IBM/BU were able to get a very good description of the band gap in the (111) direction, the ionization energy of metallic Cu, and the surface band measured in this material [18, 19]. Furthermore, with a single extra fitting parameter, the width of the interface layer close to the surface of the crystal (x1 in Fig.2.1), IBM/BU are able to obtain the correct energy of the surface state in the (111) surface and the energy of a surface resonance in the (100) surface. These states were observed experimentally by photoemission [20]. Thus, IBM/BU were able to get a consistent description of two independent experiments with a single fitting parameter.

Using this simple model for the Cu substrate IBM/BU were able to calculate the hybridization energies (or matrix elements), and have shown that these matrix elements are strongly dependent on the direction of the electron momenta, the distance of the

adatom from the surface, and the actual surface where the magnetic impurity is located. The hybridization matrix elements oscillate with distance from the surface due to the interference between the adatom localized state and the substrate states (surface and bulk) that oscillate close to the surface. IBM/BU have shown that the surface Kondo effect occurs preferentially with the surface state (when it exists) or with the bulk state at the Fermi energy that has the largest component of its momentum perpendicular to the surface.

Nevertheless, the nearly free electron approximation leads to infinite parabolic bands and when one performs the momentum sums in (1.6) they lead to divergent integrals that have to be regulated by the introduction of artificial cut-offs. As a biproduct of this free electron picture, IBM/BU observe that the distance dependence of STM tip amplitude A(R) in eq.(1.7) has oscillations and in particular IBM/BU find that the amplitude of the effect vanishes at certain distance R^* from the adatom. The vanishing of $A(R^*)$ indicates a divergence of the Fano parameter $q(R^*)$ (see eq.(1.5)). This effect is not observed in the experimental data where q(R) is nearly independent of R and A(R) is a non-vanishing function of R. These results, although inconsistent with the experimental data, are consistent with other calculations in the literature [7] where oscillations in the STM response are also obtained. Therefore, IBM/BU have found that although the nearly free electron theory is well capable of explaining the bulk of Cu and also the photoemission in Cu surfaces, it is not capable of explaining the STM response of adatoms in Cu surfaces.

Results, full model

Given the difficulties presented by simple theories of the Cu states [15], IBM/BU performed first-principle calculations of surface- and bulk-state wavefunctions on the Cu(111) surface in the presence of the scattering potential from a Co adatom, as well as their hybridization energies to the Co atom in an Anderson Hamiltonian. As the first step, BU calculated the wavefunctions of a bare Cu(111) surface. Such a surface is simulated by a supercell of twenty-one-layer slabs separated by eight vacuum layers. BU employed -- in the framework of density functional theory (DFT) – a self-consistent full-potential linearized augmented plane wave (FLAPW) method, with the exchange-correlation potential in the local density plus generalized gradient approximation (LDA+GGA). In order to further include the potential scattering from a Co adatom, BU performed another FLAPW calculation, in the local density approximation (LSDA), of seven-layer Cu slabs separated by eight vacuum layers plus Co atoms of 8-Angstrom nearest-neighbor distances on the top of the Cu surface layers. The potential difference between the Co site and the middle of two Co atoms is taken to be the scattering potential. By using the bare Cu(111) wavefuntions within the energy range of 2 eV around the Fermi surface as basis, BU diagonalized the Hamiltonian with the Co scattering potential included.

Although IBM/BU have written a C++ program to deal with the case of Co on the Cu(111) surface, it can be modified to deal with any kind of adatom in any surface. Furthermore, the program can actually deal with artificial lattices of adatoms on surfaces and can be used, in principle, to study the Kondo hole problem: this is an effect where

one eliminates one lattice site from a Kondo lattice and observes a Kondo resonance in the place of the absent adatom, that is, it is an analogue of the quantum mirage effect in a periodic system - this effect has been observed in Eigler's group [21]. Therefore, the software developed by IBM/BU can be used by STM experimentalists in order to study complicated magnetic effects and can possibly help to develop new artificial magnetic structures in metallic surfaces.

IBM/BU's computations show that the Co atom is sitting in the crystal-like regime rather than in the tunneling regime (that is, the Co adatom is strongly hybridized with the substrate), as a result the bulk states dominate the hybridization energies. This result agrees entirely with the phenomenology of recent experiments [5, 6] that find the dominance of bulk states over the surface states and raise doubts on the current interpretation of the quantum mirage in terms of surface states [4]. Moreover, IBM/BU's results lead to a new experimental proposal, namely, that the mirage effect can also occur in Cu surfaces without surface states. This prediction has not been tested experimentally so far.

To be more specific: the d-level broadening is calculated directly from the hybridization energies (without any adjustable parameters) to be 0.18eV. In fact, the STM measured Kondo temperature is TK near 50K, which, from (1.8), gives $\Delta \sim 0.2\ eV$ if one uses well established values of the parameters (eg, first principle calculations find that $\epsilon_a \sim 0.9\ eV$ [22], and photoemission results find D near 5.5 eV [23]). Therefore, the agreement between the experiment (0.20eV) and IBM/BU's first-principle calculation of the Kondo temperature (0.18eV) is excellent.

The scanning tunneling spectroscopy is calculated with the tip 2.5 Angstrom above the Co/Cu(111) surface. At further distances from the surface, IBM/BU find that the wave functions undergo an oscillatory behavior rather than a smooth exponential decay from the surface. It is known that this issue arises from GGA in the low density region because of large scaled gradients, which cause fluctuations in the exchange-correlation potential [7]. Since the usual spectroscopy experiment has a tip-surface separation of about 5 to 10 Angstroms, extrapolation of the wave function is necessary to carry the results to this distance.

In Fig.3.1 IBM/BU plot the STM signal A(R) obtained from the first principle calculation (continuous line) as compared with the free electron calculation (dashed line). One can clearly see that the oscillations as a function of R are clearly reduced and the first zero, clearly seen in the free electron case, is not present in the first principles calculation. This result dramatically indicates the importance of taking into account the full band structure in comparison with the free electron picture.
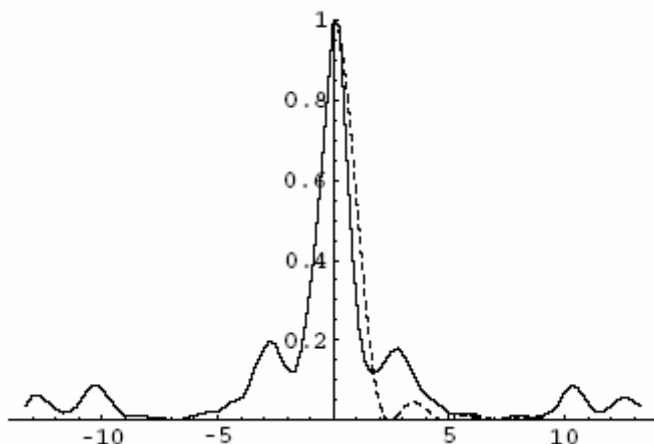
Figure 3.1: Plot of distance dependence of STM tip amplitude A(R) in the free electron picture (dashed), compared with the result of the first principle calculation (continuous).

Thus, IBM/BU have reached the conclusion that while simple theoretical models [15] are suffciently accurate to describe bulk phenomena and photoemission data, the description of STM data can only be done with the use of sophisticated ab initio band structure calculations. This result should not be completely surprising. STM experiments measure interference phenomenona that depend strongly on the tunneling path of the electrons when they move from the STM tip to the adatom. Bulk and photoemission experiments measure spectral properties that do not reflect any intereference between wavefunctions of adatoms and substrate. Therefore, the detailed form of the wavefunctions involved in a STM experiment become fundamental in the inteference effect. Nevertheless, in trying to figure out this complex phenomenona IBM/BU have developed a powerful computational tool that is able to describe artificial surface magnetism. IBM/BU hope that this tool will be helpful in the near future to explain other effects as well as a way to develop new experiments on metallic surfaces.

IBM/BU have completed ab initio studies of the Co adatom in the Cu(111) surface for different tip heights. These have been used to calculate the tunneling conductance of an STM, and to compare with recent experiments of Co impurities in the Cu(111) surface. Good quantitative agreement is found at short parallel impurity-tip distances less than 6 Angstroms. However, at larger distances, the results indicate the need for a new formulation of the problem (due to the theory giving a node in the a(R) at 7 Angstroms (see Fig. 3.1 above), which results in a divergence of the theoretical tunneling conductance at that point). Good agreement is however obtained for the normalized Fano parameters, related to the Kondo effect, at all distances.

Conclusions, Milestones and Future Work

In the three years of this collaboration the major milestones of the proposed work have been reached with great success: **milestone 1** – the mapping of the Anderson Hamiltonian for a single impurity on a surface into the surface Kondo effect, and **milestone 2** - the development of the theory for the surface Kondo effect.

Furthermore, IBM/BU have been able to explain the STM experimental data and discovered many misconceptions on the importance of surface states in understanding the STM data. On the one hand, IBM/BU's results provide support to the experimental fact that adatoms hybridize more strongly with bulk states than surface states and that the surface Kondo effect is dominated by bulk wavefunctions. On the other hand, IBM/BU's results raise doubts on current interpretation of the quantum mirage effect in terms of surface states, a result that may generate controversy in the literature, and possibly a revision of the current theoretical understanding.

More importantly, as a product of these efforts IBM/BU have developed a software based on ab initio calculations that is capable of describing the behavior of adatoms in metallic surfaces and can be used not only to help to understand current experimental data but also can provide the means to new designs for magnetic devices (the milestone 5 of this proposal).
Moreover, IBM/BU's numerical calculations can now be used to understand the Kondo lattice phase diagram (IBM/BU's milestone 4) and the amazing Kondo hole effect observed at IBM Almaden. Thus, besides completing the most important milestones IBM/BU have made major advances in order to reach the other important targets of IBM/BU's collaboration.

IBM/BU also plan to complete milestone 3, that is, the study of the two impurity Kondo problem on a surface. This is the simplest spin interacting problem with non-trivial many-body states. The only reason why this milestone was not completed yet is that IBM/BU's efforts on ab initio calculations (fundamental for the understanding of the single impurity Kondo problem) lead IBM/BU in a slightly different direction.

During the evolution of this collaboration there has been significant new breakthroughs in STM measurements that IBM/BU believe can be studied with the methods that IBM/BU have developed. One of these measurements is the Kondo hole effect in arrays of Co adatoms [21] mentioned previously. More recently the IBM Almaden group of Heinrich et al. [24] has succeeded in measuring the energy required to flip the spin of single Manganese atoms. The technique essentially measures the g-value of individual atoms with inelastic tunneling spectroscopy. This is a new technique that does not have a detailed theoretical description yet and that can produce interesting new results. This technique, for instance, can be used to study macromolecules (such as DNA) on metallic surfaces [25]. The STM can be used to first excite a standing macromolecule mode outside of the phonon continuum. Then, by inelastic tunneling spectroscopy one uses the STM to map out the location of non-linear excitations such as breathers [26].

In summary, the theoretical techniques developed by this collaboration has the potential to describe a plethora of effects observed by STM that occur at atomic scale. In this way, IBM/BU's theoretical effort not only will be able to help the understanding of the current experimental data but will also be able to open doors for new experiments and also help in the design of new magnetic devices on metallic surfaces.

Bibliography

[1] V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, and N. S. Wingreen, Science 280, 567 (1998).
[2] D. Eigler, and Schweizer, Nature 344, 524 (1990).
[3] H. C. Manoharan, C. P. Lutz, and D. M. Eigler, Nature (London) 403, 512 (2000).
[4] G. A. Fiete, and E. J. Heller, Rev. Mod. Phys. 75, 933 (2003).
[5] N. Knorr, M. A. Schneider, L. Diekhoner, P. Wahl, and K. Kern, Phys. Rev. Lett. 88, 096804 (2002).
[6] L. Limot, and R. Berndt, cond-mat/0312434.
[7] M. Plihal and J. W. Gadzuk, Phys. Rev. B 63, 085404 (2001).
[8] U. Fano, Phys. Rev. 124, 1866 (1961).
[9] J. Terso_ and D. R. Hamman, Phys. Rev. B 31, 805 (1985).
[10] P. W. Anderson, Phys. Rev. 124, 41 (1961).
[11] J. R. Schrie_er and P. A. Wol_, Phys. Rev. 149, 491 (1966).
[12] P. W. Anderson, personal communication.
[13] P. Nozieres, J. Low Temp. Phys. 17, 31 (1974).
[14] D. M. Newns and N. Read, Adv. Phys. 36, 799 (1987).
[15] C.-Y. Lin, A. H. Castro Neto, and B. A. Jones, cond-mat/0307185.
[16] G. A. Burdick, Phys. Rev. 129, 138 (1963).
[17] Basic Theory of Surface States by S. G. Davison and M. Steslicka (Oxford University Press, 1996).
[18] J. A. Knapp, F. J. Himpsel, and D. E. Eastman, Phys. Rev. B 19, 4952 (1979).
[19] S. D. Kevan, Phys. Rev. Lett. 50, 526 (1983).
[20] K. Giesen, F. Hage, F. J. Himpsel, H. J. Riess, and W. Steinman, Phys. Rev. Lett. 55, 300 (1985).
[21] D. Eigler et al., unpublished.
[22] O. Usaghy, J. Kroha, L. Szunyogh, and A. Zawadowski, Phys. Rev. Lett. 85, 2557 (2000).
[23] N. V. Smith, Phys. Rev. B 32, 3549 (1985).
[24] A. J. Heinrich, J. A. Gupta, C. P. Lutz, and D. Eigler, "Single-Atom Spin-Flip Spectroscopy", Nature, 2004 (see list of papers).
[25] J. -X. Zhu, K. O. Rassmussen, A. R. Bishop, and A. V. Balatsky, cond-mat/0407215.
[26] D. K. Campbell, S. Flach, Y. S. Kivshar, Physics Today, January 2004.

Theory, continued
2. Towards spin-polarized STM: Magnetic tunnel junctions

IBM has explored the theory of Magnetic Tunnel junctions (MTJ) with nanoscale lengths
in all three directions. With their large spin-polarized currents, such structures are
theorized to be good candidates for attachment to the end of an STM tip, with the goal of
obtaining spin-polarized STM. Theory explored the predictability of the sign and
magnitude of spin-polarized current, and the effect of interfaces on the spin current and
voltage dependences. Information on what spin currents would be produced, and at what
voltages, is critical in order for MTJ's to be an effective sensor for magnetic effects.
(The experimental construction of an MTJ on this scale for STM was supposed to occur
in the later years (years 5 and beyond) of this contract, but with the untimely end to
funding, much of this and other work proposed for the extension period have not been
performed.)

Summary of results:
IBM's theory focuses on the role of interface effects, and IBM shows, using a
combination of density functional calculations and phenomenological modeling, that
interface hybridization and disorder have a big effect, in fact changing the sign of the spin
polarized current as it passes through the interface. Calculated effective masses show key
d-electron bands with drastically lowered effective masses, in some cases less than that of
free electrons, the microscopic basis of the change in spin polarization IBM has found,
answering a scientific puzzle. Spin polarization changes across the interface in the space
of only one layer on either side, indicating possibilities of MTJ engineering with surface
layers. Theory gets good agreement with experiment, including calculated voltage-
dependent tunneling magnetoresistance as well as voltage dependence of current. IBM
will soon have a preprint which will be soon submitted to Physical Review.

Details:

Briefly, the challenges of the magnetic tunnel junction system, which has potential for
spin injectors for spintronics as well as for STM, are several fold. Why is the sign of the
spin polarized current opposite that predicted by established theory? Why does the TMR
and spin polarization drop with voltage? Can a theory be devised to explain these results
which does not resort to black box computations or seemingly ad hoc assumptions
specific to a particular materials system? IBM has explanations for the first two, and a
definite yes to the last question.
Key in IBM's explanation is IBM's postulate that interface effects, and in particular
hybridization between the metal and insulator, cause a significant change in band
structure and spin density. IBM's theory uses input from realistic, state of the art density
functional calculations to obtain effective mass and bandwidth parameters for every
relevant band in each layer. IBM uses these to obtain analytical results for the properties
of the system using a phenomenological model. IBM's density functional calculations
include the case of no explicit interface disorder (but which relaxes into such a state

nonetheless), as well as the case of one or more layers of a mix of Co and insulator atoms.

IBM finds that the LDF calculations show a finite, spin-dependent density of states at the Fermi energy in the interface insulator atoms, such that in fact the insulator near the interface becomes a magnetic semi-metal. Likewise there is a strongly altered spin asymmetry for the interface Co. This is true even for the case of no mixed layers, and simply allowing the atoms to relax into their energetically favorable positions. It becomes even more pronounced when one or two mixed layers at the interface are introduced, to mimic realistic growth conditions.

Using the extracted effective masses, IBM has calculated the spin polarized current as a function of position across the interface, and IBM finds it switches sign within a few interface layers on either side, going in one measure from -0.3 at 1 Angstrom from the interface, to 0.2 at 1 Angstrom on the insulating side. The full spin difference is not reached until several layers to either side of the interface. This sign change is consistent with the experimental observations. The explanation is that d bands are significantly changed near the interface, changing the spin balance with the s-p states (which are of opposite sign). IBM finds the spin current is mainly carried by the d bands, IBM feels settling a question of some controversy in the community.

As a function of voltage, the current density increases as expected, with the spin polarization reaching a maximum and then decreasing, as seen experimentally. IBM also calculates the TMR (Tunneling Magnetoresistance). IBM finds a positive value which decreases with voltage, also as observed experimentally. With increased voltage, the effective width of the barrier decreases, and a larger percentage of the insulating region becomes part of the interfaces, that is, semi-metallic in effect from IBM's calculations. In their model, IBM sees an increase in the tunneling from spin down, to eventually catch up to that from spin up. When up to up is equal to up to down, parallel and antiparallel configurations will be the same, giving a limiting value of TMR at very high voltages going to zero. (Other dissipative effects come to play at high voltages as well, which are not part of this model.)

IBM will soon submit a paper to Phys. Rev. Letters.
This work forms the bulk of the PhD thesis work of the Stanford graduate student Tzen Ong, whose work at IBM was funded by the contract.

Theory, continued
3. Current-induced magnetization reversal in an STM tip

As observed in the original proposal, at operating conditions, an STM produces current densities at the tip easily equal to the critical currents for magnetization reversal by spin torque. If a magnetic material, and especially a Magnetic Tunnel Junction, is to be placed on an STM tip, this is another important effect which will go into interpretation of experimental observations of spin effects with such a tip.

During the course of the contract period, IBM finished a comprehensive theory of current-induced spin torques, finding critically that the switching phase diagrams depend in a sensitive way on the local magnetic anisotropy fields in the magnetic nanolayers. In certain simple cases of axial anisotropy, the application of magnetic fields and currents results primarily in switching of the magnetization when a critical current is reached. In a

narrow sliver of phase space, in which the external magnetic field is opposite that of the magnetization, there can be precession which occurs. Since in the case of a magnetic material on an STM tip, the external magnetic field will be from the surface atoms of the sample themselves, it would need a strong atomic magnetic moment in order to achieve this time-dependent state in the tip. In the case of planar anisotropy, however, a new state is reached: that of the canted phase. That is, application of a current results in switching not from parallel to antiparallel, but from parallel (or anitparallel) to some canted relative angle of the moments. How such a canted phase could be used to optimize spin readout experimentally is still under study.

Most recently (the end period of the contract), the contract funded the work of a postdoctoral researcher at IBM, Yaroslaw Bazaliy. in the area of Spin-transfer effect in systems with continuous change of magnetization. Such a system would model, for example, an STM tip made from a block of magnetic material, large enough to produce domain walls, or other spintronic applications.

The research in 2004-2005 was concentrated on the current-induced domain wall (DW) motion. The spin-transfer action of the current in systems with continuous change of magnetization is described by the modified Landau-Lifshitz-Gilbert (LLG) equation with the spin-transfer term. The main contribution to the spin-transfer term was derived by Bazaliy, Jones, and Zhang (1998). Corrections to the main term ("non-adiabatic terms") were discussed by Tatara and Kohno (2004), Li and Zhang (2004), and Thiaville et al. (2005). Under the influence of current or magnetic field some types of domain walls move through the wire as point-like objects. For such "rigid" walls with no internal structure the complicated LLG equation in partial derivatives can be reduced to a pair of simple ordinary differential equations describing the domain wall position.

IBM's main result is the prediction of a new regime of DW motion when both magnetic field and current are acting on it. In this case there is a regime of "reversed motion" when a weak current opposing a relatively large magnetic field can overpower it and move the domain wall opposite to the field. Namely, the current can be small compared to the critical current $I_c \sim 10^8$ Amp/cm^2, and the field can be larger than the Walker breakdown field $B_w \sim 10$ Oe. This counter-intuitive effect will have a clear experimental signature. In the systems with pinning potential it will lead to the new oscillating state of the domain wall, located away from the potential minimum. Such dynamic state can be an effective building block for spintronic applications.

IBM's next result is the investigation of the AC current effect on the walls. In real wires the domain walls are always pinned by the random potential of the defects introduced during the fabrication of the wire. This random potential stops the field induced DW motion below the "propagation field" and thus diminishes the possibilities to manipulate the walls. It is shown that periodic current with right frequency can be very effective in depinning domain walls in such random pinning potentials.

Overall, these findings suggest that the interplay between the current, magnetic field, and the pinning potential in the wire can qualitatively change the motion of DW in the ways which can be useful for practical applications.

III. Listing of all publications and technical reports

(a) Papers published in peer-reviewed journals
1. A.J. Heinrich, C.P. Lutz, J.A. Gupta, D.M. Eigler, "Single-Atom Spin-Flip Spectroscopy", *Science* **306**, 466 (2004).
2. Ya. B. Bazaliy, B. A. Jones, and Shoucheng Zhang, ``Current Induced Magnetization Switching in Small Domains of Different Anisotropies", Phys. Rev. B **69**, 094421 (2004). Reprinted in the Virtual Journal of Nanoscale Science & Technology, April 5, 2004.
3. Chiung-Yuan Lin, A. H. Castro Neto, and B. A. Jones, "Microscopic theory of the single impurity surface Kondo resonance,", Phys. Rev. B **71**, 035417 (2005).
4. J.A. Gupta, C.P. Lutz, A.J. Heinrich, D.M. Eigler, "Strongly Coverage-Dependent Excitations of Adsorbed Molecular Hydrogen", *Phys. Rev.* B 71, 115416 (2005).

(b) Papers published in conference proceedings
1. Ya. B.Bazaliy, B. A.Jones, ``Magnetization rotation or generation of incoherent spin waves? Suggestions for a spin-transfer effect experiment" Physica B **329-333**, 1290 (2003).

(c) Papers presented at meetings, not published
1. "Moving Atoms: Mirages and Kondo Lattices", invited, B. Jones, Mardi Gras Symposium on Frontier Science Related to Nano, New Orleans, Feb. 8, 2002.
2. "The Science and Technology of Nanomagnetism," invited, B. Jones, Santa Clara Valley Chapter of ASM International (Materials Engineering Society), Santa Clara, CA, March 13, 2002.
3. "Nanoscience Overview," invited, B. Jones, colloquium, San Diego State University, April 15, 2002.
4. "Current-induced Magnetization Reversal in Nanostructures," invited, B. Jones, colloquium, U.C. Santa Cruz, May 10, 2002.
5. "Microscopic modeling for adatoms in Cu surfaces," invited, A. Castro-Neto and B. Jones, DARPA workshop on Spins and Spintronics, Florida, October 2, 2002.
6. "The Science and Technology of Nanoscale Systems: MTJ and Spin torques," invited, B. Jones, colloquium, University of San Francisco, Nov. 7, 2002.
7. "Nanoscience Overview," invited, B. Jones, colloquium, Cal State Univ. Northridge, Nov. 20, 2002.
10. Don Eigler, invited speaker, "Max Planck Lecture", Max Planck Institute for Solid State Research Stuttgart, Germany, May 2003. Don Eigler, invited speaker, Public Lecture, Science + Fiction – Between Nanoworld and Global Culture, Karlsruhe, Germany, May 2003.
11. Don Eigler, invited speaker, Seminar, U. Karlsruhe, Karlsruhe, Germany, May 2003.
12. Don Eigler, invited speaker, Invited Talk, Symposium on the Future of Nanotechnology in Honor of Professor Hyodo, Institute of Materials Research, Tohoku University, Sendai, Japan, May 2003.

13. Don Eigler, invited speaker, Plenary Lecture, IEEE Transducers '03 Conference, Boston, June 2003.
14. Don Eigler, invited speaker, Invited Lecture, Pan American Study Institute on Physics at the Nanometer Scale, Bariloche, Argentina, June 2003.
15. Don Eigler, invited speaker, Key Note Talk, Nano Impuls Kick Off Event, University of Twente, Twente, Netherlands, October 2003.
16. Don Eigler, invited speaker, Key Note Talk, MESA+ Institute, University of Twente, Twente, Netherlands, October 2003.
17. Don Eigler, invited speaker, Colloquium, Physics Department, Universit of California San Diego, La Jolla, October 2003.
18. Don Eigler, invited speaker, Wiener Phisikalishe Kolloquium, University of Vienna, Vienna, Austria, October 2003.
19. Don Eigler, invited speaker, Invited Talk, Royal Society Discussion Meeting – Organizing Atoms: Manipulation of Matter Below 10 nm., London, United Kingdom, October 2003.
20. Don Eigler, invited speaker, Colloquium, Physics Department, University of Linz, Linz, Austria, October 2003.
21. Don Eigler, invited speaker, Invited Talk, AIP Industrial Physics Forum, San Jose, October 2003.
22. Don Eigler, invited speaker, Plenary Lecture, International Symposium on Testing and Failure Analysis, Santa Clara, November 2003.
23. Don Eigler, invited speaker, Invited Talk, International Workshop on Smart Interconnects, Atami, Japan, November 2003.
24. Don Eigler, invited speaker, Honorary Lecture, Wulff Lecture, MIT, Boston, November 2003.
25. "Theory of STM images of Kondo systems", invited, A. Castro Neto and B. Jones, International Workshop on Quantum Mechanics at Large Scale, Banff, Canada, April 2003.
26. "Spin Coherence and Magnetization Transport in Nanometer-Scale Structures," invited, B. Jones, Conference on SpinS and Spintronics, Santa Monica, CA, Oct 15, 2003.
27. "Interpreting STM images of nanosystems of strongly correlated electrons", invited, B. Jones and A. Castro Neto, Greater Boston Area Statistical Mechanical Meeting, Boston, October 2003.
28. "Spin Transport at the Nanoscale," invited, B. Jones, Annual Meeting of the California Section of the APS, Berkeley, CA, November 15, 2003.
29. Don Eigler, invited speaker, Colloquium, Department of Physics, Nortwestern University, Evanston, March 2004.
30. Don Eigler, invited speaker, Plenary Lecture, IEEE Aerospace Conference, Big Sky Montana, March 2004.
31. Don Eigler, invited speaker, Honorary Lecture, ACS Presidential Colloquium on Nanoscience, Anaheim, March 2004.
32. Don Eigler, invited speaker, Honorary Lecture, Irish Institute of Physics Lecture Series, University of Limerick, Limerick, Ireland, April 2004.

33. Don Eigler, invited speaker, Honorary Lecture, Irish Institute of Phyiscs Lecture Series, Innauguration of University of Ulster Nanotechnology Center, University of Ulster, Jordanstown, Ireland, April 2004.
34. Don Eigler, invited speaker, Honorary Lecture, Irish Institute of Physics Lecture Series, Trinity College, Dublin, Ireland, April 2004.
35. Don Eigler, invited speaker, Seminar, Physics Department, University of Basel, Basel, Switzerland, May 2004.
36. Don Eigler, invited speaker, Seminar, Physics Department, Ecole Polytechniqe Federal Lausanne, Lausanne, Switzerland, May 2004.
37. Don Eigler, invited speaker, Seminar, Physics Department, University of Geneva, Geneva, Switzerland, May 2004.
38. Don Eigler, invited speaker, Key Note Talk, Annual Conference of the National Science and Technology Development Agency of Thailand, Bangkok, Thailand, June 2004.
39. Don Eigler, invited speaker, 6/26/2004, Invited Talk, Annual Conference of the National Science and Technology Development Agency of Thailand, Bangkok, Thailand
40. Don Eigler, invited speaker, Plenary Lecture, American Vacuum Society Annual International Symposium, Anaheim, November 2004.
41. Don Eigler, invited speaker, Seminar, Institute of Materials Research, Tohoku University, Sendai, Japan, November 2004.
42. Don Eigler, invited speaker, Invited Talk, IFCAM Forum on Electronic Properties of Interfaces and Contacts, Sendai, Japan, November 2004.
43. Don Eigler, invited speaker, Invited Talk, 1st International Symposium on Functional Organization of Nanomaterials, Tsukuba, Japan, December 2004.
44. Don Eigler, invited speaker, Key Note Talk, The European Community Conference on Images of Science: New Interactions between Science and Society, Amsterdam, The Netherlands, December 2004.
45. Don Eigler, invited speaker, Honorary Lecture, The Kronig Lecture, Technical University of Delft, Delft, The Netherlands, December 2004.
46. Don Eigler, invited speaker, Seminar, Nanotechnology Seminar, Technical University of Delft, Delft, The Netherlands, December 2004.
47. A.J. Heinrich, invited speaker, Aspen meeting, Aspen, Co, January 2004.
48. A.J. Heinrich, invited speaker, 9th International Symposium on Advanced Physical Fields, Tsukuba, Japan, March 2004.
49. A.J. Heinrich, invited speaker, Nanomaterials 2004, Wiesbaden, Germany, June 2004.
50. A.J. Heinrich, invited speaker, Gordon Conference on Nanomaterials, Tilton, NH, July 2004.
51. A.J. Heinrich, invited speaker, Gordon Conference on Nanomagnetism, Big Sky, MT, August 2004.
52. A.J. Heinrich, invited lecturer, Summer school on Molecular Electronics, Wittenberg, Germany, August 2004.
53. A.J. Heinrich, invited speaker, International Colloquium on Scanning Probe Microscopy 12, Atagawa, Japan, December 2004.

54. "Theory of STM images of Kondo systems," invited, <u>A. Castro Neto</u> and B. Jones, International Conference on "Spins in nanostructures: from Atoms to Quantum Dots to Magnets," Aspen, CO January 2004.
55. "Magnetic nanostructures and Current-Induced Magnetization Reversal," invited, B. Jones, Colloquium, U.C. San Diego Physics Dept., January 28, 2004.
56. "Theory of Magnetic nanostructures and Current-Induced Magnetization Reversal," invited B. Jones, Physics Dept. Seminar, Univ. Southern California, Los Angeles, February 20, 2004.
57. "Overview of magnetic nanostructures, and Phase Diagrams of Current-induced Magnetization Reversal," invited, B. Jones, Colloquium, U.C. Berkeley Physics Dept., May 3, 2004.
58. "Thermal effects in Current-induced Magnetization Reversal," invited, B. Jones, Seminar, Aspen Center for Physics, Aspen, CO, August 4, 2004.
59. "Challenges of Nanoscale Spins and Spin Currents," invited, B. Jones, Colloquium, Santa Clara U., November 1, 2004.
60. Don Eigler, invited speaker, Invited Talk, National Research Council Workshop on Molecular Manufacturing, Washington, February 2005.
61. Don Eigler, invited speaker, Invited Talk, Canadian Institute for Advanced Research Nanoelectronics Program, Banff, Canada, March 2005.
62. A.J. Heinrich, invited speaker, American Physical Society March Meeting, Los Angeles, March 2005.
63. "Spintronics and Magnetic Nanostructures," B. Jones, Colloquium, Cal State Fresno, February 18, 2005.
64. "Theoretical Aspects of Spintronics and Magnetic Nanostructures, Probes on the Nanoscale," invited, B. Jones, Stanford U., April 2005.

(d) Manuscripts submitted, but not published
1. Chiung-Yuan Lin, A. H. Castro Neto, and B. A. Jones, "First-principles Calculation of the Single Impurity Surface Kondo Resonance,", submitted to Phys. Rev. Lett.

(e) Technical reports submitted to ARO
1. Interim progress report, submitted 2002
2. Interim progress report, submitted 2003
3. Please see also talks given at DARPA/ARO-sponsored conferences, for which a copy of the presentation was submitted to DARPA/ARO. One such talk given at least once a year during all the course of the contract.
4. This current final report

IV. List of all participating scientific personnel, including any advanced degrees earned while on the project

At IBM:
Don Eigler - experiment
Andreas Heinrich - experiment
Chris Lutz - experiment
Bruce Melior - experiment
Barbara Jones - theory
Tzen Ong (will earn Ph.D. in 2006; B.A. Jones is his faculty advisor, via her role as Consulting Professor at Stanford University) - theory
Yaroslaw Bazaliy - theory
Amit Chattopadhyay - theory

At Boston University (theory):
Professor Antonio Castro-Neto
Chiung-Yuan Lin (earned Ph.D in 2005, faculty advisor A. Castro-Neto)

V. Report of inventions: none
VI. Bibliography: contained within section II.B1 above, See page 18

VII. Appendix: Papers and Preprints

Heinrich Gupta Lutz and Eigler Science 2004.pdf

Gupta Lutz Heinrich and Eigler PRB 2005.pdf

Lin CastroNeto and Jones PRB 2005.pdf

Bazaliy Jones and Zhang PRB 2004.pdf

Lin CastroNeto and Jones PRLsubmit.pdf